

Optical and Structural Properties of Gold/DNA Nanocomposites

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- A gold/DNA composite is a suspension of gold nanoparticles (<20 nm diam.) + DNA in aqueous solution.
- At high T, gold particles are isolated: sharp absorption line.
- At low T, DNA strands link nanoparticles into aggregate; broad absorption peak
- We have successfully modeled both aggregate freezing and change in optical properties

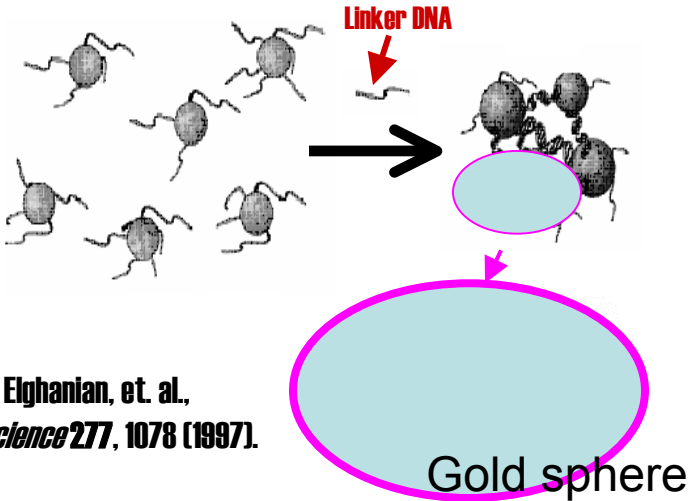
Methodology

- There are two parts to the calculation: (i) finding the structure of the composites, and (ii) computing the optical properties.
- We assume the structure forms by reaction-limited aggregation, followed by breaking of the DNA links **between** particles (“dehybridization”).

Optical props found using
“Discrete Dipole
Approximation” (DDA)

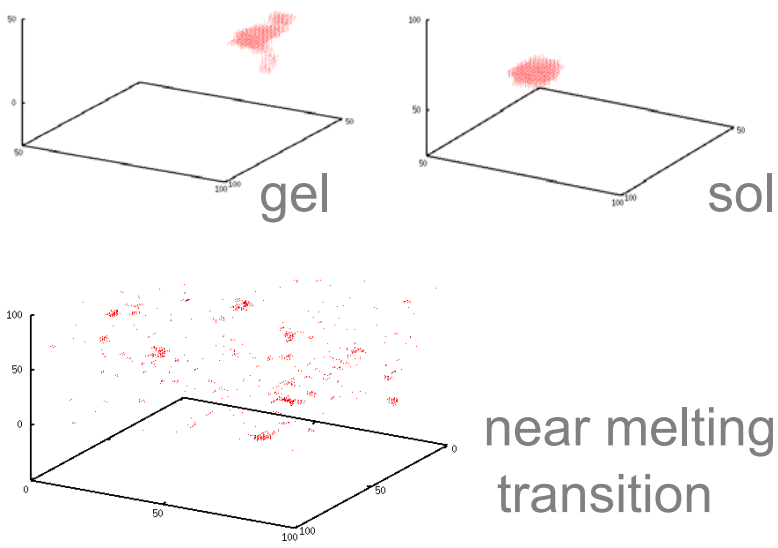
- The next slide shows
- (**upper left**) gold particles connected by DNA links;
- (**upper right**) phase diagram of aggregate;
- (**lower left**) shape of aggregate at various T; and
- (**lower right**) measured and calculated absorption at 520 nm versus T

DNA/gold nanocomposite

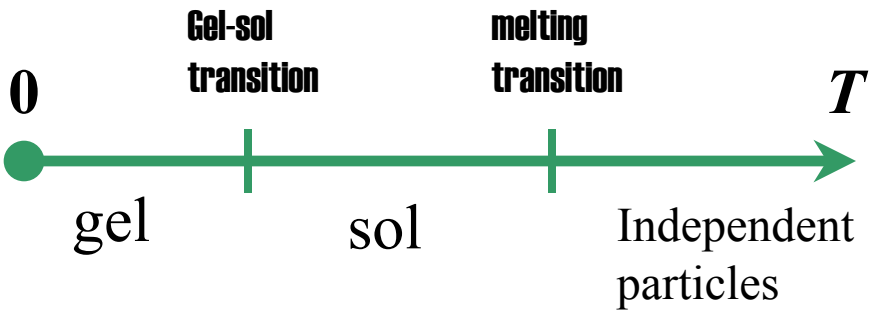


R. Elghanian, et. al.,
Science **277**, 1078 (1997).

2. Morphologies from a structural model

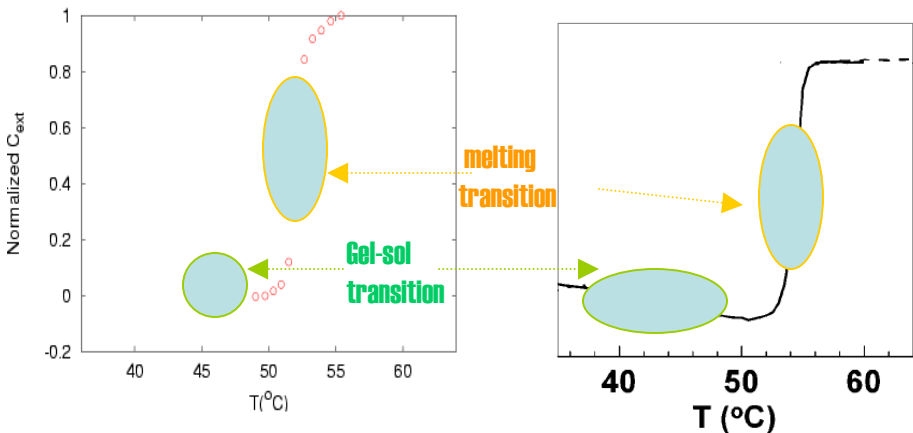


1. Expected phase diagram



3. DDA calculation of extinction cross section

Theory (left) and experiment (right)



S. Y. Park and D. Stroud, *Phys. Rev. B* (2003); R. Jin, et. al, *J. Am. Chem. Soc.* **125**, 1643 (2003).

Conclusions

- Structure and optical properties of **gold/DNA nanocomposites** can be successfully modeled
- We are now working on models which can treat optical differences between **different kinds of DNA** linked to gold particles
- Materials may be useful in **selective detection** of different organic molecules

Educational Activities of Project DMR 01-04987 - Project participants include:

- .Principal Investigator (David Stroud)
- Two postdoctoral researchers (Dr. Sung Yong Park and Dr. Hayoun Lee)
- Eight graduate students (Greg Mohler*, Eivind Almaas*, Sergey Barabash*, Wissam Al-Saidi*, Ivan Tornes, Daniel Valdez-Balderas, Kwangmoo Kim, and Kohjiro Kobayashi)
- Three international collaborators: David Bergman (Tel-Aviv Univ.), Yakov Strelniker (Bar-Ilan Univ.), Pak-Ming Hui (Chinese Univ. of Hong Kong).
- (* denotes student who has recently received Ph. D and has postdoctoral or permanent position)